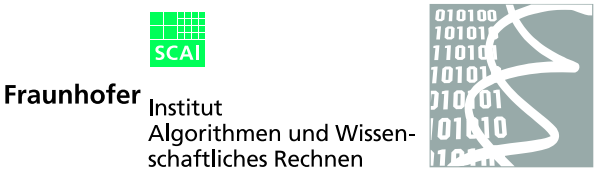
Pipeline Pilot Interface to *Hyde*

Version 3.2.5.1

User Guide

(for *Hyde* version 3.2.5 and above and Pipeline Pilot version 6.1 and above)

Edgar Derksen, Sally Hindle



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1

Quick Start Steps

1.1 Download and Import current *Hyde* Package

1. Download current "*Hyde* in PipelinePilot" package on
   http://www.biosolveit.de/download/
2. Extract *Hyde* package to a custom directory.
3. From the custom directory import all components (.xml) using PP-Client via drag and drop to your components collection.

1.2 Install *Hyde*

1. Drag and drop *Hyde* installation component from the components collection to an empty protocol.
2. Add your license for the executable of *Hyde* in the field for the parameter <Run Hyde -> on PP Server -> License Server or License File> in the Implementation tab – if your license is available from a license server, simply type in the name of the server in this format *@servername*, or if you have a license file then you may browse for it using the ... facility.
3. Run protocol once, it will result into a html report showing installation success.
4. For alternative installations and more details see chapter 3.

1.3 Create or Update Protocols

1. Drag and drop new components into a new protocol.
2. Update via a *right click drag and drop* of new component onto component reference in a protocol.
3. Now you are ready to setup the new components and run your protocol.

2

Introduction

2.1 About *Hyde*

With the advent of LeadIT 2.0 came a revolution in binding affinity prediction: Hyde Scoring. This radically new scoring function is based on pure physical principles: the hydrogen bond energy and the hydrophobic effect are both implemented in a consistent way via atomic logP increments.

The distinctly new approach in Hyde is the heavy penalization of unmet interactions: A hydrogen bond taken out of the solvent - and not having an ideal partner in the protein; or the phenyl ring that is dehydrated and put into a hydrophilic active site region. Thus, not by rewarding H-bonds but by penalizing unfavorable situations, false positives are effectively ruled out in an in silico screen.

Hyde aims at helping teams of MedChems and CompChems to decide which molecules to further pursue in a synthesis; also you could rank a series of compounds regarding their score. More application fields could be the refinement of crystal structures, or checking the effects of molecular variations on antibiotics resistances.

2.2 *Hyde* Components in Pipeline Pilot

The Hyde Scorer Component rescores docking results. First set up a Docking project within LeadIT and save as Project.fxx. Set up your Project file at parameter Hyde Project File. For each molecule at input port the component calculates a new score.

3

Installation

3.1 BioSolveIT Web Installation

The easiest way to download and install BioSolveIT packages and tools is to download and run BioSolveIT Web Installer component. Download BioSolveIT in PipelinePilot package from http://www.biosolveit.de/download. Read UserGuide within that package for further details.

Note that both PP-Client and PP-Server need web access to run BioSolveIT Web Installer. Without web access you need to follow one of the following sections in this chapter.

3.2 Using the *Hyde* Installation Component

The *Hyde* components are set by default to use a so-called auto installation of *Hyde*. This works as follows. When you run either of the *Hyde* Calculator or Similarity components (and the parameter <Run Hyde> is set to *on PP Server* and the parameter <Run Hyde-> on PP Server -> Use> is set to *FTrees Auto Installation*), they search for a *Hyde* installation in the directory:

```
<scitegic install directory>/public/bin/BioSolveIT/
```

and use this installation to run the calculation. A html report pupup shows if a *Hyde* installation is not found in this directory.

Use *Hyde* installer component to install *Hyde* prior to run calculations. In case of a default setup you don't need administrator rights to do this as it is actually Pipeline Pilot that carries out the installation and not you as a user. In special cases your system administrator prevents installations by PP and you need to ask him to install *Hyde* .

As this installation knows nothing about the licenses you may have for *Hyde*, you have to supply the license information separately. This is supplied using the parameter <Run Hyde -> on PP Server -> License Server or License File> as described above in the section 1.

The installation is carried out once only (for that *Hyde* version) and only once per server not per user. The software is available to all users once it is installed.

3.3 Using Global Variables

Use global variables as an alternative to the *Hyde* installation component decribed in section 3.2. Note that global variables will only be used if components are set to run auto installation (see. section 3.2) but no installation is done by an *Hyde* installation component yet.

Goto Administratin Portal accessible through the Server Home Page at http://localhost:9944/ if PP-Server is installed on your local machine. The Server Home Page is also available through your PP-Client in menu <Help -> Server Home Page>. Use default name: scitegicadmin and password: scitegic if you have not changed it yet. Browse to <Setup -> Globals>. Add Custom Global Protocol Properties.

Note that defining parameters within your protocol will override global variables if they are named the same. Use parameters within your protocol instead of global variables only if you want to use a custom installation for that protocol.

The first variable file_server_*Hyde*_executable: must be set to the full path of *Hyde* executable available by the PP-Server. Example:

```
C:\Program Files (x86)\BioSolveIT\FTrees\ftrees.exe
```

The second variable file_server_*Hyde*_config must be set to the full path of *Hyde* configuration. Example:

```
C:\Program Files (x86)\BioSolveIT\FTrees\config_ft.dat
```

In comparison to *Hyde* auto installation (see section 3.2) you need to check the compatibility between your defined installation and the components.

3.4 Using Custom External *Hyde* Installations

You can also use an existing external installation of the *Hyde* software. This means you also have the opportunity to use settings different to those set by default. To do this, you must already have *Hyde* installed somewhere on your system outside of Pipeline Pilot. To install *Hyde* yourself, visit the download page at BioSolveIT:
`http://www.biosolveit.de/download`
and fetch the download package for your system for the latest *Hyde* package. Follow the instructions in the package to install *Hyde* and receive your licenses. Enter the license information for *Hyde* as described in the package **and not using the parameter <Run Hyde -> on PP Server -> License Server or License File> as for the internal installation**.

To use an external installation of *Hyde*, you must change the value of the parameter <Run Hyde-> on PP Server -> Use> in the Implementation tab to *preinstalled Hyde*.

There are actually two ways to use *Hyde* with an external installation. These are by using *Hyde* installed directly on the Pipeline Pilot server , or by accessing a remote machine where *Hyde* is installed using *ssh* method. The method is selected using the parameter <Run Hyde> Both methods are covered in more detail below.

3.4.1 To Connect to an *Hyde* Installation on the Pipeline Pilot Server

The most common scenario is that you will have an installation of *Hyde* on the Pipeline Pilot server. If you choose this option, you just have to enter the path to the executable and configuration file as parameters in the Implementation tab. Pipeline Pilot will then just start *Hyde* whenever it is required by making a call to the executable that you entered.

This method is given the name *on PP Server* – On Pipelinepilot Server. You can see an example in figure 3.1.

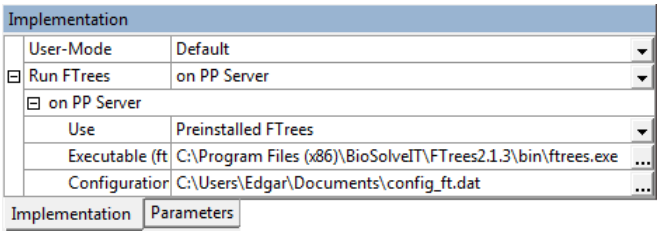

Figure 3.1: *on PP Server*: Connect to an *Hyde* Installation on the Pipeline Pilot Server

- Requirement:
  - *Hyde* is installed on the Pipeline Pilot server. You can see which machine is the Pipeline Pilot server by starting your copy of Pipeline Pilot Client on your own workstation and find the name or IP of the server shown at the bottom right of the status bar (see figure 3.2). You must find where the *Hyde* installation is *on that machine*.

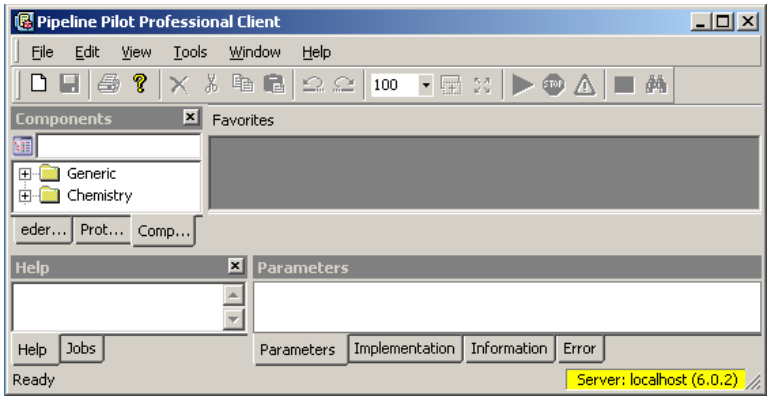

Figure 3.2: See where your Pipeline Pilot Server is installed.

- General Steps:
  1. Set <Run Hyde> to *on PP Server*
  2. Set <Run Hyde-> Use> to *Preinstalled Hyde*

3. For the parameter <Run Hyde-> on PP Server -> Executable>, enter the path to the *Hyde* installation on Pipeline Pilot server. For example:
`C:\Programs\BioSolveIT\Hyde2\bin\hyde.exe`

You can save these settings in the components.

3.4.2 To Connect to an *Hyde* Installation on a Remote Linux Server

Your existing *Hyde* installation could be on a Linux computer remote from the Pipeline Pilot server – in this case we offer an alternative so you can use the remote installation instead. Here, the calculations carried out by *Hyde* will be done on the remote Linux machine. Pipeline Pilot logs into the Linux machine using `ssh`, having copied all relevant files to the machine, and will run the calculation there, finally it needs copying back all data to the Pipeline Pilot server to continue with the pipeline.

This method is given the name *via SSH*. You can see an example in figure 3.3.

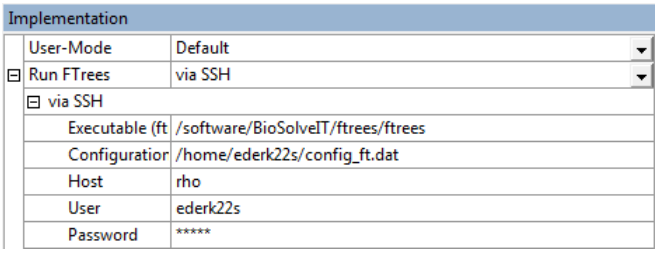

Figure 3.3: *via SSH*: Connect to an *Hyde* Installation on a Remote Linux Server via ssh

- Requirement:
  - *Hyde* is installed on a Linux machine available to the Pipeline Pilot server via `ssh`.
- General Steps:
  1. Set <Run Hyde> to *via SSH*
  2. For the parameter <Run Hyde-> via SSH -> Executable>, enter the path to the *Hyde* installation on the Linux machine. For example:
  `/software/BioSolveIT/hyde-2.0.1/bin/hyde-2.0.1`
  3. For the parameter <Run Hyde-> via SSH -> Host>, enter the Linux machine host name
- User specific steps:
  1. For the parameter <Run Hyde-> via SSH -> User>, enter the user login name for ssh on the Linux machine
  2. For the parameter <Run Hyde-> via SSH -> Password>, enter the user password for ssh on the Linux machine

3. There are more advanced options to be found under <Run Hyde-> via SSH -> Options> for more specific ssh parameters. Note the option <Run Hyde-> via SSH -> Options -> Delete Results> may be useful for trouble-shooting later.

You can save these settings in the components (be sure not to save your own user specific login details in components available to others!).

All files necessary for the *Hyde* calculation will be transferred via `scp` between the Pipeline Pilot server and ssh Linux machine. Files copied and files created the remote server are automatically deleted at the end of the job leaving no trace. However, in case the user would like to leave a copy of the calculation and result files on the Linux machine, or for trouble-shooting as mentioned above, it is possible to set a parameter to tell Pipeline Pilot not to delete these files:
<Run Hyde-> via SSH -> Options -> Delete Results> : *False*

3.5 Running *Hyde* in Parallel in Pipeline Pilot

Hyde in Pipeline Pilot takes advantage of the parallel computing options available in Pipeline Pilot to speed up longer calculations. This section tells you how to adjust the options to your system and needs. These options are only relevant to the *Hyde* Calculator and Similarity components. You will find the options in the Implementation tab, as in figure 3.4.

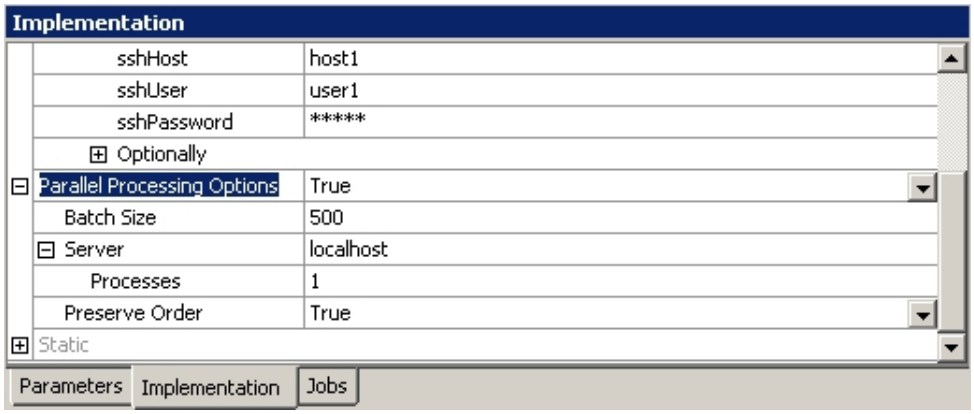

Figure 3.4: The options for tuning parallel processing are found in the Implementation tab

The most important limitation to a parallel processing calculation is the number of *Hyde* licenses that you have. If you only have a single license then parallel calculations will not be possible. Further choices in the set-up of the parallel computing computing calculation depend on the number of Pipeline Pilot licenses you have plus your choice of connection to the external *Hyde* installation (*on PP Server* or *via SSH*).

It is important to note that a balance must be achieved between the overhead caused by running several calculations instead of one and the size of the calculation – there is a lot of overhead involved in sending all the essential data to different computers and collecting the

results. For the *Hyde* Similarity component we think parallel computing will only benefit very large jobs, above 200 000 pipeline molecules or so. For the *Hyde* Calculator this number is much lower, as the calculation of feature trees is much slower. We suggest 5 000. Of course, these figures depend on the speed of your machines and network: experiment with your set-up if you intend to carry out such large calculations often. Also we advise you to read the Pipeline Pilot documentation about parallel processing to understand more fully how it works.

Note: to set up large parallel processing jobs, you will need Administrator rights to change one setting.

3.5.1 The Default Set-Up: Maintaining the Pipeline Effect

By default, the components are set to run in parallel on the *localhost* (the Pipeline Pilot server) with only one process - in essence not a parallel calculation at all! These are the default values, below we give an explanation for these settings.

- *on PP Server* method of connection to the external *Hyde* installation (*Hyde* is installed on the Pipeline Pilotserver).
- <Parallel Processing Options> is set to *True*.
- <Server> set to *localhost*
- <Processes> 1

The idea behind using these settings is to enhance the pipeline effect for the *Hyde* components, not to run a true parallel calculation. By choosing these settings, Pipeline Pilot is forced to collect the incoming pipeline molecules into sets. As soon as one set is complete (a set contains the number of molecules set by the parameter <Batch Size>) Pipeline Pilot starts the calculations for the component. Hence, the *Hyde* components are already running while the pipeline continues to deliver molecules, saving time. As soon as all molecules have arrived, the pipeline continues. Note that the <Batch Size> parameter for both components is set more with this idea in mind, rather than for a true parallel calculation.

If the option <Parallel Processing Options> is set to *False*, all molecules must arrive at the *Hyde* component before a calcuation is started. This means a little performance may be gained by avoiding the overhead required to split the pipeline into batches, however, the *Hyde* component may only start when it has all molecules and the pipeline can only begin again once the *Hyde* component is finished.

Even if you do not have a multi-processor server, or do not wish to calculate in parallel, we recommend you still keep these default options to enhance the pipeline effect as explained above.

3.5.2 Running in Parallel on the Pipeline Pilot Server

You may have a multi-processor machine as your Pipeline Pilot server. If you also have the appropriate number of Pipeline Pilot and *Hyde* licenses the simplest way to start a parallel

calculation is to raise the number of processes to the number of processors of the machine.

You could also have more than one Pipeline Pilot server available in your network. If so, you can enter a list of the server names at the parameter <Server>. Below that, for the parameter <Processes> enter a list of the number of processes each server should receive. The lists are both comma separated and must be in corresponding order. Remember to adjust also the <Batch Size> accordingly.

Note: the path to the external installation of *Hyde* must be same on all servers!

3.5.3 Running in Parallel on a Remote Linux Cluster

We have developed an implementation in the components whereby a large cluster can be incorporated to run *Hyde* jobs, without them having to be Pipeline Pilot servers. However, it must be a Linux cluster and the components must use the ssh method. You must also have enough *Hyde* licenses available to the cluster.

The settings in the Implementation tab must be made as for running the ssh method, with two important changes. Instead of one <Run Hyde -> via SSH -> Host>, enter a comma separated list of the host names in the Linux cluster. Then, you must choose how many batchs in total you want the job to be split into and enter this total in the <Processes> parameter. Remember to change the <Batch Size> to fit with the number of processes.

Figure 3.5 may help clarify how the method works.

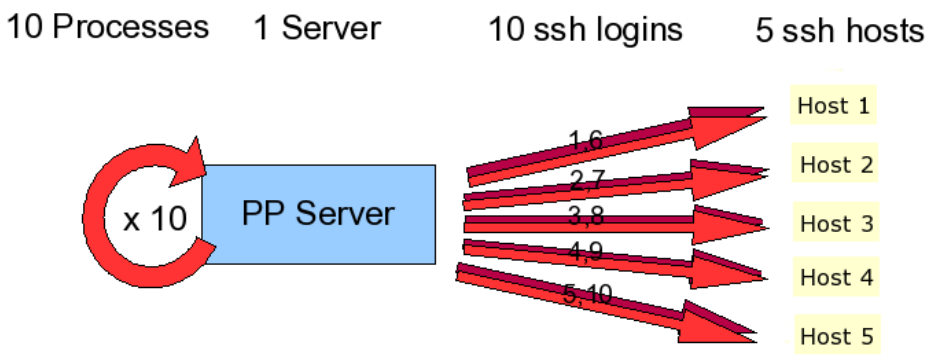

Figure 3.5: The method of parallel processing on Linux clusters in the *Hyde* components. The Pipeline Pilot server is given 10 processes. The 10 processes start an ssh job respectively, distributed amongst the ssh hosts.

The Pipeline Pilot server will run with the number of processes given in <Processes>. However, in this case the processes the server receives are not the *Hyde* calculations themselves but instructions for starting the ssh jobs. The server iterates through its 10 jobs each time spawning an ssh job on a Linux host. Beware that the Pipeline Pilot server does not know how many processors the Linux hosts have so make sure you choose the number of

<Processes> to fit the number of Linux hosts and their number of processors respectively – be careful not to overload the Linux hosts.

Figure 3.6 shows the detailed settings required to set up the calculation as in figure 3.5.

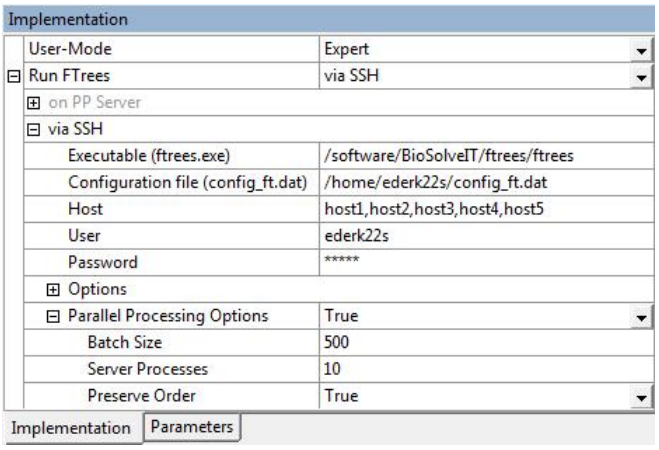

Figure 3.6: The options for parallel processing for the example shown in figure 3.5 would look similar to these

As you may already have realised, you could enter more than one Pipeline Pilot server at the <Server> parameter (along with another entry for number of <Processes> as a comma separated list) to execute a doubly parallel calculation!

Note: to get this method to work you will need to change the maximum number of processes per Pipeline Pilot server. The Pipeline Pilot Client will let you enter any number for the <Processes> parameter and does not warn you if this number is above the maximum.

Changing the maximum number requires Administrator rights! The number of processes per Pipeline Pilot server is usually restricted to the number of processors of the server. You must override this maximum to be able to set the number of processes you want for your parallel calculation. In the above example, the maximum must be set to 10 or more. Take the following steps:

- Go to the 'Scitegic Server Home Page', for example, via the Help menu in your Pipeline Pilot client.
- Click on 'Pipeline Pilot Administration Portal' and log in with the Administrator user name and password.
- In the last field of the table ('Maximum number of simultaneous parallel processing subprotocols allowed') change the value, click 'Save' and log out again.

3.5.4 Example Scenarios and Required Settings

ssh/ops	*ops*
Parallel Processing Options	False
Number of PP servers in list	1
Number of ssh Hosts in list	-
Number of Processes	-
Behavior	The calculation will run as one complete job on the Pipeline Pilot server
ssh/ops	*ssh*
Parallel Processing Options	False
Number of PP servers in list	-
Number of ssh Hosts in list	1
Number of Processes	-
Behavior	The calculation will run as one complete job on the ssh host
ssh/ops	*ops*
Parallel Processing Options	True
Number of PP servers in list	1
Number of ssh Hosts in list	-
Number of Processes	1
Behavior	(Default) Induces the 'pipeline' effect: the job will run in chunks on the server processor(s)
ssh/ops	*ops*
Parallel Processing Options	True
Number of PP servers in list	1
Number of ssh Hosts in list	-
Number of Processes	>1
Behavior	A true parallel effect: the job will be run in chunks on the server processors
ssh/ops	*ops*
Parallel Processing Options	True
Number of PP servers in list	4 (each with two processors)
Number of ssh Hosts in list	-
Number of Processes	2,2,2,2
Behavior	A true parallel effect: the job will run in chunks in parallel split across 8 processors
ssh/ops	*ssh*
Parallel Processing Options	True
Number of PP servers in list	1
Number of ssh Hosts in list	5 (each with 2 processors)
Number of Processes	10
Behavior	A true parallel effect: the job will run in chunks in parallel split across 10 processors

3.6 Uninstallation

Use the *Hyde* installer component to uninstall previous *Hyde* versions by switching Parameter "Uninstall Previous Versions" to "True".

Use BioSolveIT Uninstaller component to uninstall all *Hyde* versions.

Note that this kind of deinstallation only removes *Hyde* versions installed by *Hyde* installer component or BioSolveIT web installer component.

4

Trouble Shooting

4.1 Problems connecting to the external installation

Other most commonly seen problems with *Hyde* in Pipeline Pilot is with the connection to the external *Hyde* installation. For one thing, *Hyde* itself must be correctly installed on the system independently of Pipeline Pilot – it is essential first to make sure this is the case (especially to make sure that *Hyde* can locate the licenses). Once *Hyde* runs fine on your system, the remaining key task is to make sure the paths to the executable and configuration file are correct within the Pipeline Pilot components.

The simplest test to check whether *Hyde* is running OK in Pipeline Pilot is to set up the workflow shown in section **??** with just 10 molecules or so. If something is amiss with the connection to the external installation, you will see an error message box pop up. Check the paths to the executable or to the configuration file. If it seems *Hyde* could be started but not run, the problem almost always lies either with the path to the configuration file or with licenses not being found. If *Hyde* runs OK independently from Pipeline Pilot then it is likely to be the path to the configuration.

When the error messages pop up, they may contain an HydeError in the error message box, as in figure 4.1.

Go to the 'Jobs' tab below the Protocol workspace and check under the last run job for a file called 'HydeComponent Debug' – as in figure 4.2. Clicking on the link brings up HTML report with input and output data in a browser.

A correctly started *Hyde* job outputs the following header: if there is a problem you will see some of this header and the point where the problem occurs:

```
 _____________________________________________________
/                                                     /
/                    F T R E E S                      /
/       Feature-based molecular similarity finder     /
/                                                     /
/=====================================================/
/                                                     /
/  Version:  2.0.2  (11.08.08)                       /
/  Modules: [PVM] [FFS]                               /
/                                                     /
/ written by:  Matthias Rarey, Marc Zimmermann,       /
```

```
       /               Sally Hindle, Robert Fischer             /
      /                                                         /
     / copyright by: BioSolve IT GmbH, FhG -SCAI               /
    /                Sankt Augustin, Germany                  /
   / for further information mail hyde-info@biosolveit.de /
  /_____________________________________________________/
 Additional copyright notes:
   getline library: (C) 1993 by Chris Thewalt
   PVM library: (C) 1997 by University of Tennessee, Knoxville TN
 >> Hyde configuration file '/software/BioSolveIT/Hyde/hyde2.0.1/
    config_ft.dat' loaded.

 >> Licensed modules: Hyde [PVM] [FFS]
 >> PVM status: no pvm daemon, running sequential.
 >> Scripts are executed in sequential mode; start PVM for parallel mode.
 >> SETTINGS = '/software/BioSolveIT/hyde2.0.1/static_data/hyde_settings.dat'
    loaded.
 >> CHEMPAR  = '/software/BioSolveIT/hyde2.0.1/static_data/chempar.dat' loaded.
 >> CONTACT  = '/software/BioSolveIT/hyde2.0.1/static_data/contact_ft.dat' loaded.
 >> TRANSFORM = '/software/BioSolveIT/hyde2.0.1/static_data/transform.dat' loaded.
 >> GRAPHIC  = '/software/BioSolveIT/hyde2.0.1/static_data/graphic_ft.dat' loaded.
...
```

4.2 Problems using the *ssh* Method

You may also experience problems using the *ssh* login, for example, the user name is unknown or the host is not found.

4.3 Further help and BioSolveIT PDF Reporter

More complicated errors may arise during the running of *Hyde*. Again though, the errors will be collected and as much information shown as possible. If you are familiar with *Hyde* you may want to take a look at all the output of the job yourself to see if you can recognize the problem. In this case, you can look in the temporary folders Pipeline Pilot sets up internally to find the output, or if you are working with the *ssh* method, set the parameter <Run Hyde -> via SSH -> Options -> Delete Results> to *False* so that you may then find the files retained on the *ssh* host: these will be in the directory set under the ssh parameter <Run Hyde -> via SSH -> Options -> Temp Path> (see the help text associated with this parameter to find its default value) – essentially a cryptically named folder whose name begins with the date and time of the job!

If you still do not know what is causing the errors, write down as much information as possible relating to your installation scheme. You can also create a PDF Report unsing BioSolveIT PDF Reporter component which summarizes installation data into one pdf file. Send all the information to:

support@biosolveit.de

Figure 4.1: An error box reporting that the *Hyde* exe exited with error.

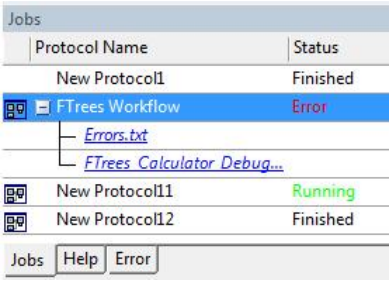

Figure 4.2: The full error report can be found in the 'Jobs' tab.

5

Tips and Tricks

5.1 Other Significant Parameters in the *Hyde* Components

For detailed documentation of all parameters for all components, refer to the documentation you find in the *Help* area of the Pipeline Pilot window.

We list here particularly interesting parameters: those that greatly influence the workflow or change the outcome of calculations, or those that may help you understand what is happening in the components.

5.1.1 <Has Same File System>

*Hyde*Calculator/Similarity : Implementation : <Run Hyde-> via SSH -> Options -> Has Same File System>

Normally, for an *ssh* job, Pipeline Pilot must first copy all the data required by Hyde to the <Run Hyde -> via SSH -> Host> using scp. This is time consuming. It is possible that the Pipeline Pilot Server and <Run Hyde -> via SSH -> Host> actually share the same file system rendering the scp process unnecessary. Select True if the Pipeline Pilot Server and <Run Hyde -> via SSH -> Host> share the same File System - no copying of data is necessary. Selecting False means Pipeline Pilot copies all the data to and back from the <Run Hyde -> via SSH -> Host> – this is just a little slower but will always still work. Leave the parameter set to False if you are uncertain!

5.2 Accessing Other Domains within Pipeline Pilot

Often in house data or even your own working data are accessible from a windows computer via a domain (a path starting for example 'z:\...' or '\\...') which you cannot find from within Pipeline Pilot. That means you must first literally transfer the data to the Pipeline Pilot Server itself.

If you are using a Linux Pipeline Pilot server, this hint does not apply.

To get around this problem and make the Pipeline Pilot working environment much more flexible you can allow users access to domains – you need Administrator rights to be able to do this! Also check first that you should change these settings as they may have already been set to fit the current environment.

- Go to the 'Scitegic Server Home Page', for example, via the Help menu in your Pipeline Pilot client.
- Click on 'Pipeline Pilot Administration Portal' and log in with the Administrator user name and password.
- In the Security tab go to Authentification.
- For the 'Authentification Method' choose 'DOMAIN' and a set of parameters will appear.
- Enter the domain name in the field 'Domain' and choose 'Full' for 'Impersonation'
- Choose 'DOMAIN' for 'Retrieve Groups' and leave 'Limit access to listed domains' set to 'No'
- click 'Save' and log out again.

After you have done this you will need to enter your domain login details when you start the Pipeline Pilot Client.

Bibliography